

=> screen 963  
L1 SCREEN CREATED  
=> screen 1821 OR 1822 OR 1823 OR 1824

L2 SCREEN CREATED  
=>  
Uploading C:\Program Files\Stnexp\Queries\09676487-b.str

L3 STRUCTURE UPLOADED

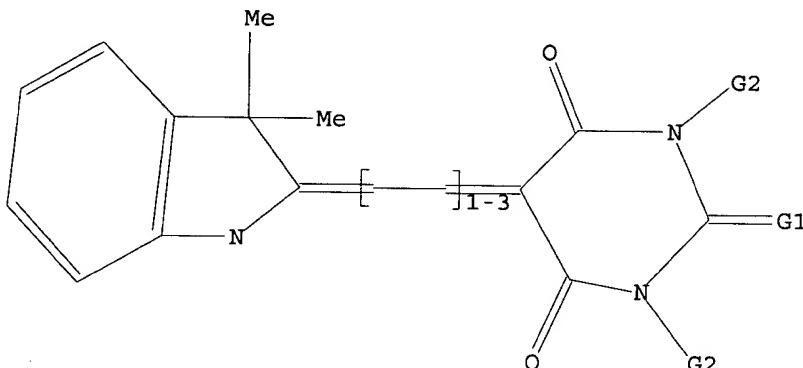
=> que L3 AND L1 AND L2

L4 QUE L3 AND L1 AND L2

=> d

L4 HAS NO ANSWERS

L1 SCR 963  
L2 SCR 1821 OR 1822 OR 1823 OR 1824  
L3 STR



G1 O, S

G2 H, Cb, Hy, Ak, Ph

G3 H, Ak

Structure attributes must be viewed using STN Express query preparation.  
L4 QUE ABB=ON PLU=ON L3 AND L1 AND L2

=> s 14 sss sam  
SAMPLE SEARCH INITIATED 11:18:56 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 5 TO ITERATE

100.0% PROCESSED 5 ITERATIONS 4 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 5 TO 234  
PROJECTED ANSWERS: 4 TO 200

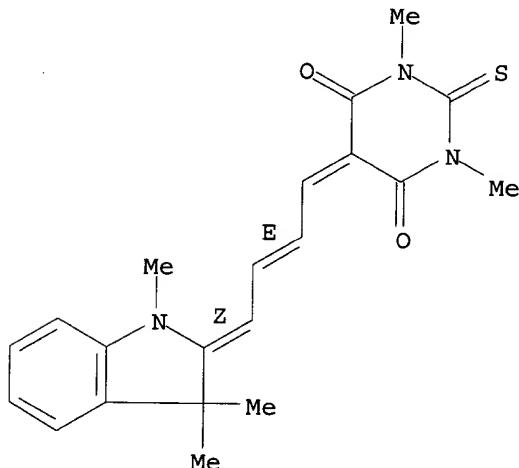
L5 4 SEA SSS SAM L3 AND L1 AND L2

=> d

STN  
Search

LS ANSWER 1 OF 4 REGISTRY COPYRIGHT 2003 ACS  
RN 521060-32-2 REGISTRY  
CN 4,6(1H,5H)-Pyrimidinedione, 5-[(2E,4Z)-4-(1,3-dihydro-1,3,3-trimethyl-2H-indol-2-ylidene)-2-butenylidene]dihydro-1,3-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C21 H23 N3 O2 S  
SR CA  
LC STN Files: CA, CAPLUS

Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1957 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

=> FIL CAPLUS HCAPLUS USPATFULL USPAT2  
COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE ENTRY	TOTAL SESSION
3.28	3.49

FILE 'CAPLUS' ENTERED AT 11:20:37 ON 26 JUN 2003  
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FILE 'USPATFULL' ENTERED AT 11:20:37 ON 26 JUN 2003  
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FILE 'USPAT2' ENTERED AT 11:20:37 ON 26 JUN 2003  
CA INDEXING COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

=> d his

(FILE 'HOME' ENTERED AT 11:18:10 ON 26 JUN 2003)

FILE 'REGISTRY' ENTERED AT 11:18:22 ON 26 JUN 2003  
L1 SCREEN 963  
L2 SCREEN 1821 OR 1822 OR 1823 OR 1824  
L3 STRUCTURE uploaded  
L4 QUE L3 AND L1 AND L2  
L5 4 S L4 SSS SAM

FILE 'CAPLUS, HCAPLUS, USPATFULL, USPAT2' ENTERED AT 11:20:37 ON 26 JUN 2003

=> s 15  
L6 8 L5

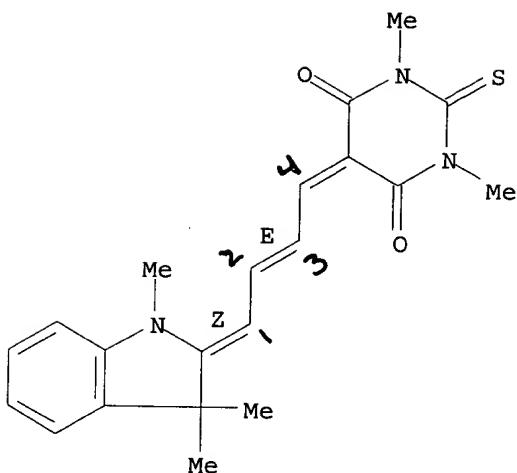
=> duplicates remove 16  
DUPLICATE PREFERENCE IS 'CAPLUS, HCAPLUS'  
KEEP DUPLICATES FROM MORE THAN ONE FILE? Y/(N) :n  
PROCESSING COMPLETED FOR L6  
L7 4 DUPLICATE REMOVE L6 (4 DUPLICATES REMOVED)

=> d 17 1-4 ibib abs hitstr

L7 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2003 ACS DUPLICATE 1  
ACCESSION NUMBER: 2003:193710 CAPLUS  
DOCUMENT NUMBER: 138:350727  
TITLE: Solvent-sensitive dyes to report protein conformational changes in living cells  
AUTHOR(S): Toutchkine, Alexei; Kraynov, Vadim; Hahn, Klaus  
CORPORATE SOURCE: Department of Cell Biology, Scripps Research Institute, La Jolla, CA, 92037, USA  
SOURCE: Journal of the American Chemical Society (2003), 125(14), 4132-4145  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Covalent attachment of solvent-sensitive fluorescent dyes to proteins is a powerful tool for studying protein conformational changes, ligand binding, or posttranslational modifications. We report here new merocyanine dyes that make possible the quantitation of such protein activities in individual living cells. The quantum yield of the new dyes is sharply dependent on solvent polarity or viscosity, enabling them to report changes in their protein environment. This is combined with other stringent requirements needed in a live cell imaging dye, including appropriate photophys. properties (excitation >590 nm, high fluorescence quantum yield, high extinction coeff.), good photostability, minimal aggregation in water, and excellent water solv. The dyes were derivatized with iodoacetamide and succinimidyl ester side chains for site-selective covalent attachment to proteins. A novel biosensor of Cdc42 activation made with one of the new dyes showed a 3-fold increase in fluorescence intensity in response to GTP-binding by Cdc42. The dyes reported here should be useful in the prepn. of live cell biosensors for a diverse range of protein activities.

IT 521060-32-2P  
RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)  
(solvent-sensitive dyes to report protein conformational changes in living cells)  
RN 521060-32-2 CAPLUS  
CN 4,6(1H,5H)-Pyrimidinedione, 5-[(2E,4Z)-4-(1,3-dihydro-1,3,3-trimethyl-2H-indol-2-ylidene)-2-butenylidene]dihydro-1,3-dimethyl-2-thioxo- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



$R_{1,2} = Me$

$Q_3 = S$

$m = 2$

$R^h = Me$

$R^{d-g} = H$

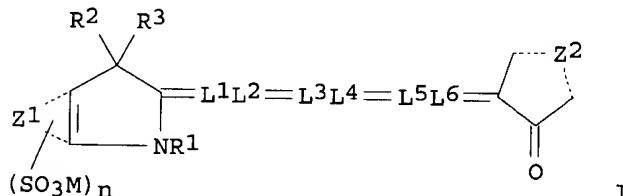
REFERENCE COUNT:

72

THERE ARE 72 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2003 ACS DUPLICATE 2  
 ACCESSION NUMBER: 1996:693723 CAPLUS  
 DOCUMENT NUMBER: 125:312364  
 TITLE: Silver halide photographic materials containing hexamethinemericyanine compounds  
 INVENTOR(S): Sakurada, Masami; Oono, Shigeru  
 PATENT ASSIGNEE(S): Fuji Photo Film Co Ltd, Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 33 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08211552	A2	19960820	JP 1995-15010	19950201
PRIORITY APPLN. INFO.:			JP 1995-15010	19950201
GI				



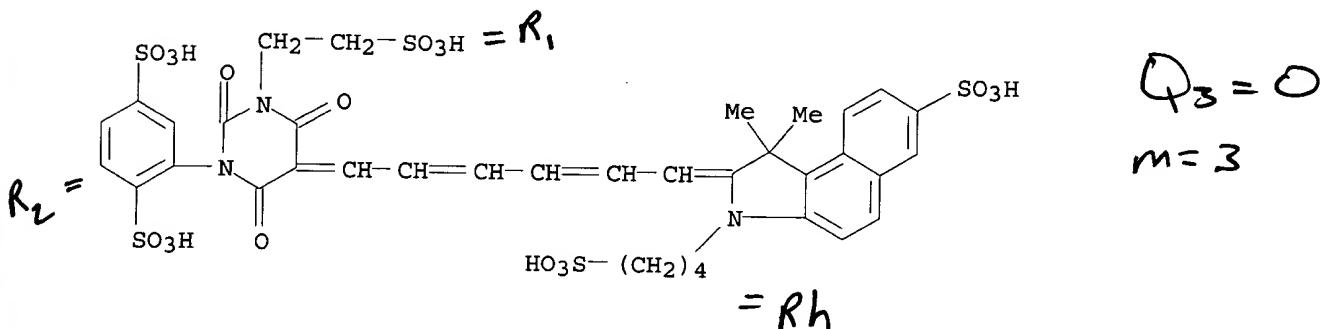
AB The title materials comprise a hydrophilic colloid layer contg.  $\text{R}^h$  hexamethinemericyanine compd. I [ $Z_1$  = nonmetal atoms required to form a benzo-condensed or naphtho-condensed ring;  $M = H$ , atoms or metal atom forming a monovalent cation;  $n = 1-3$ ;  $R_{1-3} =$  (substituted) alkyl;  $L_{1-6}$  (substituted) methine group, the adjacent substituents may be condensed to form a 5- or 6-membered ring;  $Z_2$  = atoms required to form a (substituted) heterocycle selected from pyrazolidinedion, isooxazolone, pyrazolopyridone, barbituric acid, pyridone, rhodanine]. The compds. are stable and water-sol. and provide photog. materials showing improved decoloring properties without adverse effects on the photog. properties.

IT 183272-29-9

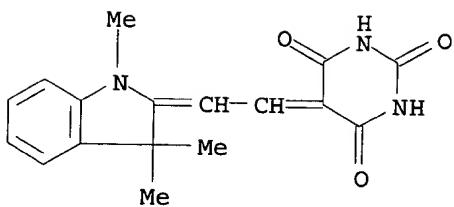
RL: DEV (Device component use); USES (Uses)  
(Ag halide photog. materials contg. hexamethinemericocyanine compds.)

RN 183272-29-9 CAPLUS

CN 1,4-Benzenedisulfonic acid, 2-[5-[6-[1,3-dihydro-1,1-dimethyl-7-sulfo-3-(4-sulfobutyl)-2H-benz[e]indol-2-ylidene]-2,4-hexadienylidene]tetrahydro-2,4,6-trioxo-3-(2-sulfoethyl)-1(2H)-pyrimidinyl]-, pentapotassium salt (9CI) (CA INDEX NAME)



L7 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2003 ACS DUPLICATE 3  
ACCESSION NUMBER: 1996:640204 CAPLUS  
DOCUMENT NUMBER: 125:278576  
TITLE: Molecular hyperpolarizabilities of barbituric acid and cyclobutene-1,2-dione derivatives. Electronic and steric effects  
AUTHOR(S): Cho, Bong Rae; Je, Jong Tae; Lee, Seung Jae; Lee, Sang Hae; Kim, Hyun Soo; Jeon, Seung Joon; Song, Ok-Keum; Wang, C. H.  
CORPORATE SOURCE: Department of Chemistry, Korea University, Seoul, 136-701, S. Korea  
SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1996), (10), 2141-2144  
PUBLISHER: Royal Society of Chemistry  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB A series of merocyanine dyes contg. various donors and barbituric acid and cyclobutene-1,2-dione moieties as the acceptors have been synthesized and their first-order hyperpolarizabilities  $\beta$ . were detd. The  $\beta$ . values of the barbituric acid derivs. increase as the strength of the donor is increased from 4-(dimethylamino)phenyl to trimethylindolinyl to benzothiazolinyl, apparently due to the gradual decrease in the bond length alteration from a large pos. value to an optimum one by a stronger donor. In contrast, the  $\beta$ . values for the cyclobutene-1,2-dione derivs. decrease with the same variation of the donors even though the cyclobutene-1,2-dione is a poorer acceptor than the barbituric acid moiety. The results have been attributed to the electron-donating ability of the donors and the increased distortion of the chromophores from planarity.  
IT 93818-94-1P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (hyperpolarizabilities of merocyanines from barbituric acid and cyclobutenediones)  
RN 93818-94-1 CAPLUS  
CN 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-[(1,3-dihydro-1,3,3-trimethyl-2H-indol-2-ylidene)ethylidene]- (9CI) (CA INDEX NAME)



$m=1$   
 $Q_3=O$   
 $R_{1,2}=H$   
 $R_h=Me$   
 $R_d=g=H$

L7 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2003 ACS  
 ACCESSION NUMBER: 1963:426202 CAPLUS  
 DOCUMENT NUMBER: 59:26202  
 ORIGINAL REFERENCE NO.: 59:4716e-g  
 TITLE: Stereochemical factors affecting optical sensitization  
 AUTHOR(S): Anderson, G. de W.  
 CORPORATE SOURCE: Imp. Chem. Inds. Ltd., Manchester, UK  
 SOURCE: Sci. Phot., Proc. Intern. Colloq., Liege (1962), 1959,  
 487-511  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 GI For diagram(s), see printed CA Issue.  
 AB The formation of polymeric forms (J aggregates contg. at least 150 mols.) of sensitizing dyes in Ag halide emulsions is studied. The positions of the absorption max. in MeOH and in the emulsion are given for a large no. of merocyanines. Symmetry of the terminal groups and, in general, redn. of the no. of possible stereoisomers, promotes the J aggregation. Electronic rather than structural symmetry is an essential, but not the sole requirement. Malononitrile dimethinemerocyanines with 2 stereo forms show J-band aggregation. N,N'-Diethylthiobarbituric acid dimethinemerocyanines show aggregation only when a single isomer is possible. The no. of stereoisomers can be limited by enclosing the polymethine chain in a cyclic system. Even highly similar d and I forms increase this no. and prevent J-band sensitization. A new 4,7'-quinocyanine of structure I is described.  
 IT 93818-94-1, Barbituric acid, 5-[2-(1,3,3-trimethyl-2-indolinylidene)ethylidene]-  
 (photographic sensitization by, stereoisomerism and)  
 RN 93818-94-1 CAPLUS  
 CN 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-[(1,3-dihydro-1,3,3-trimethyl-2H-indol-2-ylidene)ethylidene]- (9CI) (CA INDEX NAME)

